Journal of Solid and Fluid Mechanics (JSFM), 15(1): 1-4, 2025

Shahrood University of Technology

Journal of Solid and Fluid Mechanics (JSFM)

DOI: **10.22044/jsfm.2025.14657.3869**

Manufacturing Engineering of Iran

Determining the Reaction Rate of Molybdenite Powder and Exploring the Effect of Temperature on It.

Abdollah Shabani Shahrbabaki[1], **Vali Kalantar**[2]

[1]PhD Student, Yazd university, Yazd, Iran.
[2]Assoc. Prof., Yazd university, Yazd, Iran.
*Corresponding author: Vkalantar@yazd.ac.ir

Received: 2024/10/06…. Revised: 2025/16/02 Accepted: 2025/23/03

Abstract

In this work, the reaction rate of molybdenite powder is determined, and the effects of temperature on the reaction rate and reaction time are investigated. The particle temperature is calculated by solving the heat transfer equation, including convection, conduction, and radiation terms. The particle diameter is assumed to be 100 µm and the porosity is 50%. The results show that the particle temperature reaches the fluidized bed temperature in 365 seconds, and the reaction time is around 5000 seconds. According to the results, during the time interval from 500 seconds to 1800 seconds, the temperature of the particles is higher than 600°C, which causes sintering of molybdenum trioxide. The fluidized bed temperature must be decreased, and the gas velocity should be increased to prevent sintering. The results are in good agreement with the experimental data. This article is part of a study on the design and construction of a fluidized bed furnace. For the first time in the country, a pilot-scale fluidized bed roaster has been built based on these results.

Keywords: Reaction Rate; Temperature; Fluidized Bed; Roasting; Molybdenite.

1. Introduction

The fluidized bed technique is extensively used for oxidizing, heating, and drying powdered materials, finding applications in diverse fields such as chemical, food, pharmaceutical, and mining sectors. The fluidized bed offers numerous advantages, including high heat transfer, uniform moisture removal, and reduced drying time.

The reaction rate is one of the most important parameters affecting the oxidation of powder particles, which depends on behavior of particles in the gas phase. Many studies have been conducted on the oxidation temperature of molybdenite particles and reaction rate [۵-۱]. According to the results of Xiao et al. [۶], the oxidation reaction of molybdenite begins at 450°C, and at temperatures above 500°C, the reaction rate significantly increases. Modeling based on the unreacted core was performed, showing that initially, the chemical reaction in the gas phase has an apparent activation energy of 123.180 kJ/mol. However, in the final stages, the reaction becomes diffusion-controlled, with diffusion within the particles determining the reaction rate. Wilkomirski [۷] demonstrated that, for particle sizes ranging from 35 to 55 microns, oxidation is a first-order reaction following the unreacted core model, controlled by activation energy of 104 kJ/mol.

Abdel-Rehim [۸] investigated the oxidation of molybdenite, showing that the reaction starts at 360-370°C and increases significantly at 500-570°C. Molybdenum oxide melts at 770-795°C and boils at 1150-1280°C. It was also determined that the sintering of molybdenum oxide starts at 600-650°C.

The authors of this article have also conducted research on two-phase flow, particle combustion, and heat transfer between particles and gas [۱۴-۹], which can be utilized for the design of a fluidized bed furnace.

Since the present study was aimed at constructing a furnace for the oxidation of molybdenum sulfide in the Shahrbabak Copper Complex located in Kerman Province, the reaction rate and oxidation reaction completion time were determined based on the conditions and specifications of the molybdenum sulfide powder used in the molybdenum plant of the Sarcheshmeh Copper Complex. A pilot-scale fluidized bed furnace was subsequently designed and built accordingly.

2. Mathematical Modelling

The geometry of the problem corresponds to the schematic diagram in Figure 1.

The heat transfer equation between a particle and the bed fluid is derived by taking into account conduction, convection, radiation, as well as heat production terms. Due to the particles' small diameter, the Biot number is below 0.1, enabling the neglect of temperature variations within the particle and the assumption of a uniform particle temperature.

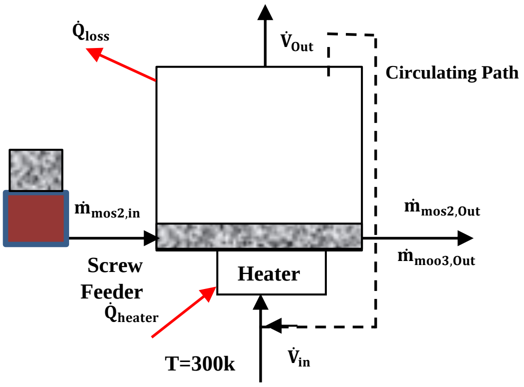

Figure 1. Schematic diagram

The energy conservation equation for the particles is formulated and represented as follows:

$$n_{pv}m_p c_p v_{px}\frac{dT_p}{dx} = \frac{d}{dx}\left(k_{sx}\frac{dT}{dx}\right) + A_{pv}h\left(T_g - T_p\right) + k_{Rad}\varepsilon\sigma\left(T_W^4 - T_p^4\right) + \dot{m}_p n_{pv}\left(-\Delta H_{Reaction}\right) \qquad (1)$$

k_sx, the coefficient of effective solid heat conduction in the x-direction, in case where the gas temperature varies in the x-direction, can be derived using the following equation:[15]

$$k_{sx} = k_e^0 + 0.5 Pr Re_{px} k_a - k_{ax}\varepsilon_g \qquad (2)$$

3. Reaction rate modeling

According to Abdel-Rehim's findings [8], if powder particles remain at a temperature below the reaction threshold—ranging from 360 to 400°C—for an extended period, the oxidation reaction proceeds at a slow rate. A dense layer of molybdenum oxide develops on the particle's surface, inhibiting oxygen penetration into the particle. Conversely, when the particles are rapidly exposed to a furnace temperature exceeding 450°C, a porous oxide layer forms on their surfaces, allowing the reaction to progress to completion in the gas phase, as described by the equation below [8]:

$$kt = \left[1 - (1 - \propto)^{1/3}\right] \qquad (3)$$

In this equation, k is the reaction rate constant and ∝ is the fraction of molybdenite that has been oxidized. The constant k depends on the reaction temperature and, for a temperature of 600 °C, is equal to $k = 1.85 \times 10^{-4}$. In the present study, since the powder particles are introduced into the furnace at ambient temperature, it takes time for them to reach a temperature equal to that of the bed fluid. Therefore, the reaction rate remains zero until the particle temperature reaches the reaction onset temperature. Once the particle temperature reaches the onset temperature, the reaction rate starts increasing from zero, and as the temperature rises to the bed fluid temperature, the reaction rate also increases. In order to calculate the heat generation term in the heat transfer equation and given that the particle temperature is not constant along the furnace, the dependence of the reaction rate on temperature must be determined. Based on reaction rate modeling according to the Arrhenius model, the constant **A** is derived using the following formula [16]:

$$k = A \exp[-E_a/(RT)] \qquad (4)$$

Reaction constant (k) is plotted in figure 2.

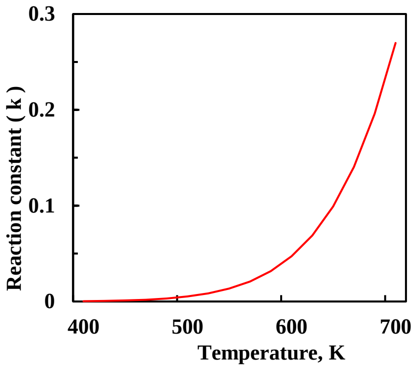

Figure 2. Reaction constant per temperature

According to Abdel-Rehim's findings [8], the activation energy is 123,180 kJ/mol, and the constant A is 1,106,700. Using the reaction rate constant (k) and Equation 1, the fraction of molybdenite that has reacted can be determined. To compute the mass of the reactant within the time interval dt, the differential d∝ must first be calculated. By differentiating Equation 3 and simplifying it, d∝ is expressed in the following form:

$$d \propto = 3k(1 - \propto)^{2/3} dt \qquad (5)$$

By multiplying the input mass flow rate by d∝, the reaction mass rate is obtained as follows:

$$d\dot{m} = \dot{m} \times d \propto \qquad (6)$$

4. Results and Discussion

Based on the calculated reaction rate results, the source term in the heat transfer equation can be determined, enabling the analysis of the temperature profile and reaction rate along the furnace. As illustrated in Figure 3, the particle enters the furnace at an initial temperature of 300 K, rises to the bed fluid temperature of 793 K within 365 seconds, and shortly thereafter, due to heat generation from the reaction, reaches its peak temperature.

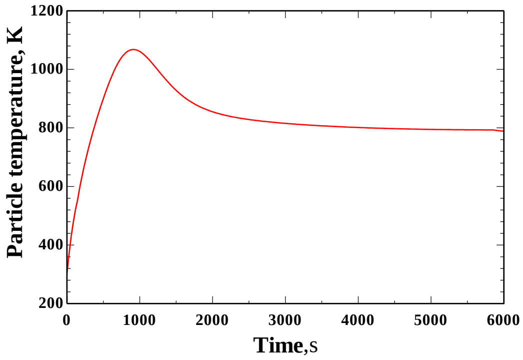

Figure 3. Particle temperature per time

The most important parameter calculated in this study is the reaction rate, which is plotted in Figure 4.

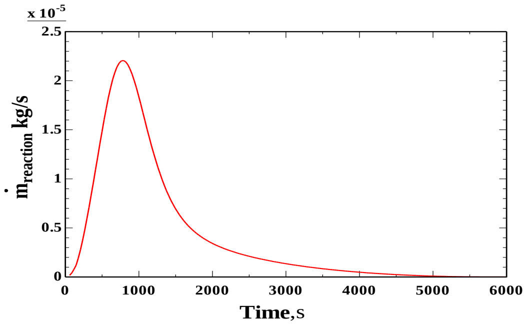

Figure 4. Reaction Rate per time

According to Figure 4, the reaction rate is initially zero due to the low temperature of the particles. As the particle temperature increases, the reaction rate also rises, reaching its maximum value after 780 seconds.

To validate the obtained results, the reaction time derived from the equations used in this study is compared with experimental results and is plotted in Figure 5.

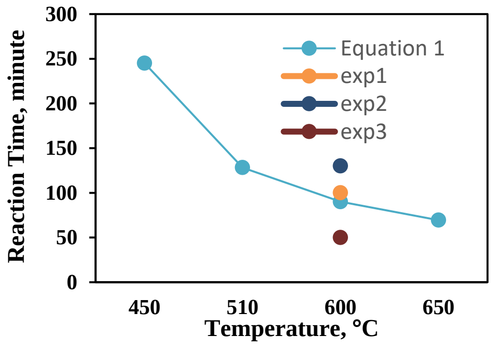

Figure 5. Reaction time of this work and experimental results(exp1 [17], exp2[18], exp3 [19])

Based on the findings of this study, a pilot-scale fluidized bed furnace has been constructed at the molybdenum plant of the Shahr-e Babak Copper Complex (Figure 6).

Figure 6. pilot-scale fluidized bed was constructed as part of this research.

5. Conclusions

In this study, the reaction rate of molybdenum powder, with particle diameters of 100 microns and a porosity of 50%, was determined across various temperatures. From this data, the heat generation term as a function of time was calculated. The reaction rate began at zero, increased gradually, peaked after 780 seconds, and then sharply decreased to zero. The initial increase in the reaction rate resulted from the rising particle temperature, while its rapid decline was attributed to two factors: the decreasing particle temperature and the reduced amount of unreacted powder. The total reaction time for these particles was found to be 5,000 seconds, with the particle temperature reaching the bed fluid temperature after 365 seconds.

Additionally, it was observed that between 500 and 1,800 seconds, the particle temperature exceeded the permissible oxidation range. To prevent the agglomeration of powder particles, the bed fluid temperature must be reduced while the fluid velocity should be increased to improve the convective heat transfer coefficient.

Based on the results of this study, a pilot-scale fluidized bed furnace was designed and constructed at the Shahr-e Babak Copper Complex.

6. References

[1] H.I.C. Peláez, M. Cortés-Rodríguez, R. Ortega-Toro, Storage stability of a fluidized-bed agglomerated spray-dried strawberry powder mixture, *F1000Research*, 12 (2023) 1174.

[2] J. Liu, L. Wang, G. Wu, Sintering Behavior of Molybdenite Concentrate During Oxidation Roasting Process in Air Atmosphere: Influences

of Roasting Temperature and K Content, *Molecules*, 29(21) (2024) 5183.

[3] J. Heo, S. Baek, K. Kurniawan, S. Han, Y. Kim, H. Park, J. Seo, Optimizing rotary kiln operations for molybdenite concentrate oxidation roasting to produce molybdic trioxide, *Chemical Engineering Journal Advances*, 20 (2024) 100642.

[4] A.A. Shaikh, J. Bhattacharjee, P. Datta, S. Roy, A comprehensive review of the oxidation states of molybdenum oxides and their diverse applications, *Sustainable Chemistry for the Environment*, (2024) 100125.

[5] W. Zhang, K. Wang, Y. Tian, L. Liao, H. Liu, High hydrogen evolution reaction performance of MoS2 nanosheets with sulfur vacancies synthesized from natural molybdenite, *Journal of Materials Science*, (2025) 1-12.

[6] X.-b. Li, W. Tao, Q.-s. Zhou, T.-g. Qi, Z.-h. Peng, G.-h. Liu, Kinetics of oxidation roasting of molybdenite with different particle sizes, *Transactions of Nonferrous Metals Society of Chin*a, 31(3) (2021) 842-852.

[7] I. Wilkomirsky, A. Otero, E. Balladares, Kinetics and reaction mechanisms of high-temperature flash oxidation of molybdenite, *Metallurgical and Materials Transactions B*, 41(1) (2010) 63-73.

[8] A. Abdel-Rehim, Thermal analysis and X-ray diffraction of roasting of Egyptian molybdenite, *Journal of Thermal Analysis and Calorimetry*, 57 (1999) 415-431.

[9] M. Bidabadi, N. Moallemi, A. Shabani, M. Abdous, Analysis of size distribution and ignition temperature effects on flame speeds in aluminium dust clouds, Proceedings of the Institution of Mechanical Engineers, Part G: *Journal of Aerospace Engineering*, 224(1) (2010) 113-119.

[10] M. Bidabadi, A. Shabani, An analytic model for flame quenching distance in aluminum dust suspensions, *Australian Journal of Basis and Applied Sciences*, 2(4) (2008) 1058-1067.

[11] M. Bidabadi, A. Shabani Shahrbabaki, M. Jadidi, S. Montazerinejad, An analytical study of radiation effects on the premixed laminar flames of aluminium dust clouds, Proceedings of the Institution of Mechanical Engineers, Part C: *Journal of Mechanical Engineering Science*, 224(8) (2010) 1679-1695.

[12] A.S. Shahrbabaki, R. Abazari, Perturbation method for heat exchange between a gas and solid particles, *Journal of applied mechanics and technical physics*, 50(6) (2009) 959-964.

[13] A.S. Shahrbabaki, V. Kalantar, S.H. Mansouri, Analytical and numerical considerations of the minimum fluidization velocity of the molybdenite particles, *Computational Particle Mechanics*, (2022).

[14] A. Shahrbabaki, M. Dodangeh, Particle temperature distribution in a dust flame, Proceedings of the Institution of Mechanical Engineers, Part C: *Journal of Mechanical Engineering Science*, 224(2) (2010) 363-367.

[15] M.A. Izquierdo Barrientos, *Heat transfer and thermal storage in fixed and fluidized beds of phase change materials*, (2014).

[16] J.H. Espenson, Chemical kinetics and reaction mechanisms, *Citeseer*, 1995.

[17] W. Lu, G.-h. Zhang, D. Jie, K.-c. Chou, Oxidation roasting of molybdenite concentrate, *Transactions of Nonferrous Metals Society of China*, 25(12) (2015) 4167-4174.

[18] S. Kan, K. Benzeşik, M.Ş. Sönmez, O. Yücel, Roasting of Molybdenite Concentrates in Pilot Scale Rotary Furnace.

[19] T. Marin, T. Utigard, C. Hernandez, Roasting kinetics of molybdenite concentrates, *Canadian Metallurgical Quarterly*, 48(1) (2009) 73-80.